CONTENTS

Special Issue: Electron Density and Chemical Reactions

Preface	i
The LCAO representation of the first order density matrix in non-orthogonal basis sets: a note	
I. Mayer (Budapest, Hungary)	1
An observable-based interpretation of electronic wavefunctions: application to 'hypervalent' molecules	
J. Cioslowski (Tallahassee, FL, USA) and P.R. Surján (Budapest, Hungary) An ab initio study of hydrogen abstraction from propane by the CN radical	9
J.J.W. McDouall (Manchester, UK) Efficient new methods for the determination of integrated atomic properties via atom specific electron density functions based on subsets of selected localized molecular orbitals and the reduction of the space of the primitives	35
R. Glaser and B.L. Harris (Columbia, MO, USA)	45
The use of the charge density to investigate chemical reactions; the displacement of methy chloride by fluoride ion	
K.E. Laidig (Cambridge, UK) A simple quantum mechanical elementary act model for S _N 2 nucleophilic substitution in aqueous solutions	93
D.E. Khoshtariya (Tblisi, Georgia)	131
Similarity and complementarity in chemistry	
R.F.W. Bader, P.L.A. Popelier and C. Chang (Hamilton, Ont., Canada)	145
Properties of atoms in molecules: protonation at carbonyl oxygen	
T. Slee (Waterloo, Ont., Canada) and R.F.W. Bader (Hamilton, Ont., Canada)	173
Description of chemical reactions in terms of the properties of the electron density	
E. Kraka and D. Cremer (Gothenburg, Sweden)	189
Topological electron density analysis of halogen-substituted phosphirenes	
S.M. Bachrach (DeKalb, IL, USA)	207
The molecular electron density distribution. Meeting place of X-ray diffraction and quantum chemistry intermediate between theory and experiment	
D. Feil (Enschede, The Netherlands)	221
Experimental electron density and electrostatic properties of peptides by high resolution X- ray diffraction	
C. Lecomte, N. Ghermani, V. Pichon-Pesme and M. Souhassou (Nancy, France)	241
R.G. Pearson (Santa Barbara, CA, USA)	261
Applications of calculated local surface ionization energies to chemical reactivity J.S. Murray, T. Brinck and P. Politzer (New Orleans, LA, USA)	271
Ab initio study of the effect of external perturbations in the dissociation of CH ₃ Cl M. Solà, E. Carbonell, A. Lledós, M. Duran and J. Bertran (Bellaterra, Spain)	283
Some comments concerning the use of static charge distributions for predicting chemical reactivity	
J.P. Ritchie (Los Alamos, NM, USA)	297
Degenerate Li–H exchange in first-row hydrides: a charge density analysis P.V. Sudhakar, K. Lammertsma (Birmingham, AL, USA) and P. von R. Schleyer	
(Erlangen, Germany)	309
Quantum topological study on the structure of chemical bonds in alkylidenecarbene and lithiofluoro-carbenoid	
SJ. Zheng, LP. Meng, XH. Cai (Shijiazhuang, China) and TH. Tang	327
(Toronto, Ont., Canada)	321

The electron density and chemical bonding in organic compounds by X-ray diffraction V.G. Tsirelson and R.P. Ozerov (Moscow, Russia)	335
A topological analysis of bond activations in alcohols and fluoroalkanes by protonation in the gas phase	
M. Esseffar, M. El Mouhtadi (Marrakech, Morocco), V. López and M. Yáñez (Madrid, Spain)	393
Experimental vs. theoretical topological properties of charge density distributions. An application to the L-alanine molecule studied by X-ray diffraction at 23 K	
C. Gatti, R. Bianchi, R. Destro and F. Merati (Milan, Italy)	409
Shapes of independent atoms and chemical deformation densities of second-row molecules	
W.H.E. Schwarz, H.L. Lin, S. Irle and J.E. Niu (Seigen, Germany)	435
Electron density as the basic variable: a divide-and-conquer approach to the ab initio computation of large molecules	
W. Yang (Durham, NC, USA)	461
Announcement	481
Erratum	483
Author index	485
Subject index	487

